



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:09 AM UTC

PDB ID : 1EW2 / pdb_00001ew2
Title : CRYSTAL STRUCTURE OF A HUMAN PHOSPHATASE
Authors : Le Du, M.H.; Stigbrand, T.; Taussig, M.J.; Menez, A.; Stura, E.A.
Deposited on : 2000-04-21
Resolution : 1.82 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

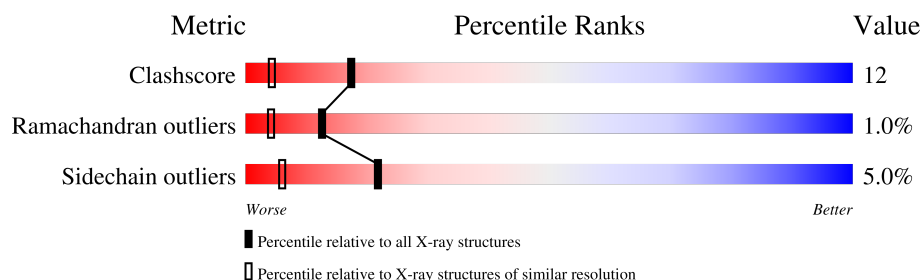
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	513	69% 18% 5% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	1005	-	X	X	-

2 Entry composition [i](#)

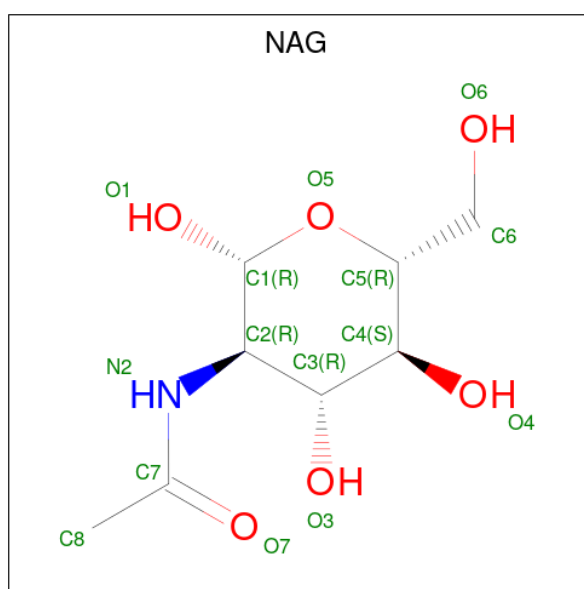
There are 6 unique types of molecules in this entry. The entry contains 4277 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3652	2285	651	698	18			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

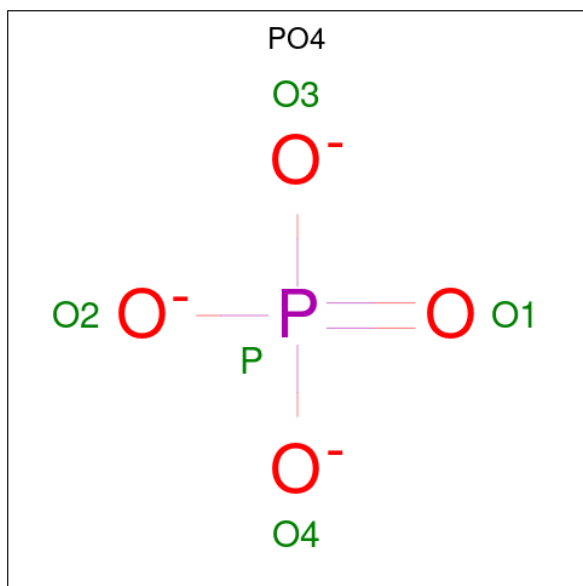
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	602	Total	O	0	0
			602	602		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.80Å 114.50Å 106.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.00 – 1.82	Depositor
% Data completeness (in resolution range)	(Not available) (22.00-1.82)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4277	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAG, PO4, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	3/3733 (0.1%)	1.93	101/5066 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	358	HIS	ND1-CE1	-6.47	1.26	1.32
1	A	478	PRO	C-O	-5.76	1.20	1.25
1	A	479	PRO	N-CD	5.59	1.55	1.47

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	THR	N-CA-CB	23.30	145.87	110.45
1	A	125	ARG	CD-NE-CZ	13.94	143.91	124.40
1	A	358	HIS	ND1-CE1-NE2	12.83	121.23	108.40
1	A	82	THR	CB-CA-C	-11.54	89.57	109.65
1	A	472	THR	N-CA-C	-11.37	95.20	110.55
1	A	262	VAL	O-C-N	-11.29	108.46	122.57
1	A	82	THR	CA-CB-OG1	10.54	125.41	109.60
1	A	431	THR	N-CA-CB	-10.49	94.19	110.56
1	A	301	ARG	CD-NE-CZ	10.02	138.43	124.40
1	A	180	GLN	CB-CG-CD	9.72	129.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	HIS	CA-CB-CG	-9.59	104.21	113.80
1	A	107	PHE	CA-CB-CG	9.26	123.06	113.80
1	A	358	HIS	CE1-NE2-CD2	-9.14	99.86	109.00
1	A	472	THR	CA-CB-CG2	8.85	125.55	110.50
1	A	472	THR	CA-CB-OG1	-8.73	96.50	109.60
1	A	478	PRO	O-C-N	8.65	125.29	121.31
1	A	474	CYS	N-CA-C	-8.45	99.38	110.53
1	A	72	ASP	CA-CB-CG	8.24	120.84	112.60
1	A	432	HIS	CE1-NE2-CD2	8.14	117.14	109.00
1	A	309	PHE	CA-CB-CG	7.88	121.69	113.80
1	A	453	GLN	CB-CG-CD	7.80	125.86	112.60
1	A	66	GLU	CA-C-N	-7.66	117.08	122.59
1	A	66	GLU	C-N-CA	-7.66	117.08	122.59
1	A	249	ASN	OD1-CG-ND2	-7.65	114.95	122.60
1	A	474	CYS	CA-C-N	-7.63	111.80	123.17
1	A	474	CYS	C-N-CA	-7.63	111.80	123.17
1	A	120	GLN	OE1-CD-NE2	-7.58	115.02	122.60
1	A	357	ASP	CB-CG-OD1	7.33	135.26	118.40
1	A	60	LYS	CA-C-N	-7.33	110.79	122.95
1	A	60	LYS	C-N-CA	-7.33	110.79	122.95
1	A	262	VAL	CA-C-O	-7.18	111.81	120.78
1	A	135	ARG	NE-CZ-NH1	-7.07	114.43	121.50
1	A	432	HIS	CG-CD2-NE2	-6.81	100.39	107.20
1	A	310	VAL	O-C-N	6.78	129.61	123.03
1	A	474	CYS	CA-C-O	-6.74	114.05	121.87
1	A	478	PRO	CA-C-O	6.71	125.73	120.90
1	A	469	GLU	CA-C-O	-6.60	111.11	120.16
1	A	263	THR	N-CA-CB	6.60	121.64	110.49
1	A	361	VAL	CA-C-N	6.57	131.45	122.19
1	A	361	VAL	C-N-CA	6.57	131.45	122.19
1	A	60	LYS	O-C-N	-6.57	113.14	121.74
1	A	154	ALA	N-CA-C	6.55	118.08	111.07
1	A	60	LYS	CA-C-O	-6.53	113.45	121.67
1	A	224	GLY	CA-C-N	6.50	126.16	119.92
1	A	224	GLY	C-N-CA	6.50	126.16	119.92
1	A	255	GLN	CB-CG-CD	6.50	123.64	112.60
1	A	430	GLU	CA-C-O	6.47	128.41	121.55
1	A	180	GLN	CA-CB-CG	6.39	126.88	114.10
1	A	260	PRO	O-C-N	-6.30	115.31	123.06
1	A	471	TYR	CA-C-N	-6.29	108.11	121.32
1	A	471	TYR	C-N-CA	-6.29	108.11	121.32
1	A	270	GLU	O-C-N	6.23	126.20	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	HIS	CA-CB-CG	-6.13	107.67	113.80
1	A	260	PRO	N-CA-C	-6.09	101.70	111.38
1	A	135	ARG	CA-CB-CG	-6.08	101.93	114.10
1	A	62	LYS	N-CA-C	6.06	119.32	110.17
1	A	316	ASP	CA-CB-CG	-6.05	106.55	112.60
1	A	261	SER	N-CA-CB	6.04	120.70	110.49
1	A	92	SER	CB-CA-C	-6.00	100.66	110.85
1	A	357	ASP	CB-CG-OD2	-5.97	104.67	118.40
1	A	359	SER	CA-C-N	5.93	131.82	122.21
1	A	359	SER	C-N-CA	5.93	131.82	122.21
1	A	316	ASP	N-CA-CB	-5.89	101.16	109.94
1	A	205	LYS	N-CA-C	5.89	118.48	111.71
1	A	92	SER	N-CA-C	5.87	117.76	111.36
1	A	42	ASP	CB-CG-OD2	5.84	131.84	118.40
1	A	255	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	51	ALA	CA-C-O	-5.78	114.43	120.55
1	A	171	ASP	O-C-N	-5.75	114.91	122.39
1	A	42	ASP	CA-CB-CG	-5.74	106.86	112.60
1	A	276	TYR	N-CA-C	-5.67	102.64	110.35
1	A	192	SER	N-CA-CB	-5.63	101.80	110.42
1	A	167	ASN	OD1-CG-ND2	5.60	128.20	122.60
1	A	312	GLY	N-CA-C	-5.59	99.94	113.18
1	A	320	HIS	CE1-NE2-CD2	5.49	114.49	109.00
1	A	432	HIS	ND1-CE1-NE2	-5.47	102.93	108.40
1	A	8	ASN	CA-C-N	5.42	125.50	119.32
1	A	8	ASN	C-N-CA	5.42	125.50	119.32
1	A	358	HIS	CG-ND1-CE1	-5.41	100.10	109.30
1	A	260	PRO	CB-CA-C	5.40	118.05	110.98
1	A	130	ILE	N-CA-C	5.37	116.31	108.58
1	A	263	THR	CA-C-O	-5.36	112.84	120.51
1	A	469	GLU	CB-CA-C	5.30	120.61	110.17
1	A	249	ASN	CB-CG-OD1	5.30	131.39	120.80
1	A	429	GLU	O-C-N	5.30	129.73	123.27
1	A	8	ASN	CA-C-O	5.25	123.21	119.32
1	A	51	ALA	O-C-N	5.25	127.68	122.12
1	A	255	GLN	CG-CD-NE2	5.25	124.27	116.40
1	A	311	GLU	CA-C-O	5.22	126.07	120.38
1	A	370	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	241	ARG	N-CA-C	5.20	117.92	109.24
1	A	395	ASN	CB-CG-ND2	5.19	124.18	116.40
1	A	230	GLY	CA-C-O	5.12	124.73	119.00
1	A	202	GLY	CA-C-O	-5.11	116.66	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ASP	O-C-N	5.11	126.46	121.66
1	A	204	ARG	CB-CA-C	-5.10	102.32	110.79
1	A	89	VAL	O-C-N	5.06	125.83	121.12
1	A	306	PHE	O-C-N	5.05	129.33	122.96
1	A	314	ARG	NE-CZ-NH1	-5.04	116.47	121.50
1	A	430	GLU	O-C-N	-5.03	116.63	122.81
1	A	450	HIS	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	468	LEU	Mainchain
1	A	82	THR	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3652	0	3539	90	0
2	A	14	0	13	1	0
3	A	2	0	0	0	0
4	A	2	0	0	0	0
5	A	5	0	0	2	0
6	A	602	0	0	28	4
All	All	4277	0	3552	90	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:HD21	6:A:1556:HOH:O	1.16	1.32
1:A:23:ALA:O	1:A:26:LEU:HD22	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ALA:O	1:A:26:LEU:CD2	2.26	0.84
1:A:162:HIS:H	1:A:189:GLN:HE22	1.23	0.83
1:A:135:ARG:HD2	1:A:469:GLU:HA	1.64	0.78
1:A:383:ARG:HG2	6:A:1328:HOH:O	1.87	0.73
1:A:82:THR:HG23	6:A:1576:HOH:O	1.88	0.73
1:A:402:LYS:HE3	1:A:407:PRO:HB3	1.70	0.72
1:A:29:ALA:HB2	6:A:1603:HOH:O	1.90	0.72
1:A:135:ARG:HH11	1:A:135:ARG:HG3	1.59	0.66
1:A:259:ASP:OD2	1:A:260:PRO:O	2.14	0.66
1:A:135:ARG:HD3	6:A:1605:HOH:O	1.96	0.65
1:A:469:GLU:HA	6:A:1605:HOH:O	1.96	0.64
1:A:82:THR:CB	6:A:1576:HOH:O	2.44	0.63
1:A:82:THR:CG2	6:A:1576:HOH:O	2.46	0.62
1:A:472:THR:O	1:A:473:ALA:HB3	2.01	0.61
1:A:82:THR:CG2	1:A:90:PRO:HG3	2.31	0.60
1:A:472:THR:OG1	1:A:473:ALA:N	2.28	0.60
1:A:453:GLN:HG2	6:A:1046:HOH:O	2.02	0.60
1:A:469:GLU:CB	1:A:470:PRO:CD	2.80	0.59
1:A:26:LEU:CD2	6:A:1556:HOH:O	2.00	0.58
1:A:135:ARG:HG3	1:A:135:ARG:NH1	2.19	0.58
1:A:10:ASP:HB2	6:A:1558:HOH:O	2.04	0.58
1:A:92:SER:OG	5:A:1005:PO4:P	2.62	0.58
1:A:137:LYS:HE2	1:A:195:ASP:HB3	1.86	0.57
1:A:431:THR:HG23	1:A:432:HIS:O	2.04	0.57
1:A:95:THR:HG22	1:A:455:GLN:HE22	1.71	0.56
1:A:5:GLU:HA	6:A:1469:HOH:O	2.05	0.55
1:A:472:THR:HG22	6:A:1379:HOH:O	2.05	0.55
1:A:302:ASN:ND2	1:A:304:ARG:H	2.04	0.55
1:A:353:LEU:HD12	1:A:458:ILE:HG23	1.88	0.54
1:A:204:ARG:HG2	1:A:268:LEU:HB3	1.88	0.54
1:A:135:ARG:NH1	6:A:1132:HOH:O	2.24	0.54
1:A:172:ALA:HA	1:A:228:LEU:HD22	1.90	0.54
1:A:135:ARG:CD	1:A:469:GLU:HA	2.38	0.53
1:A:242:GLN:OE1	6:A:1601:HOH:O	0.53	0.53
1:A:82:THR:HG21	1:A:90:PRO:HG3	1.90	0.53
1:A:99:TYR:CD1	1:A:100:LEU:HG	2.44	0.53
1:A:243:GLY:O	1:A:262:VAL:O	2.28	0.52
1:A:153:HIS:HD2	6:A:1115:HOH:O	1.90	0.52
1:A:135:ARG:HH11	1:A:135:ARG:CG	2.18	0.52
1:A:162:HIS:H	1:A:189:GLN:NE2	2.02	0.52
1:A:260:PRO:O	1:A:261:SER:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:THR:O	1:A:392:LEU:HD21	2.10	0.52
1:A:472:THR:O	1:A:473:ALA:CB	2.58	0.52
1:A:391:LEU:C	1:A:392:LEU:HD22	2.34	0.52
1:A:469:GLU:CA	6:A:1605:HOH:O	2.55	0.52
1:A:439:VAL:HG21	1:A:458:ILE:HD11	1.92	0.51
1:A:92:SER:HG	5:A:1005:PO4:P	2.33	0.51
1:A:26:LEU:HD23	6:A:1346:HOH:O	2.09	0.51
1:A:162:HIS:HE1	6:A:1079:HOH:O	1.93	0.51
1:A:82:THR:HG21	1:A:358:HIS:HB3	1.92	0.50
1:A:251:THR:O	1:A:255:GLN:HG3	2.10	0.50
1:A:111:GLY:O	1:A:162:HIS:HD2	1.94	0.50
1:A:411:GLU:HG2	6:A:1566:HOH:O	2.12	0.49
1:A:288:LEU:O	1:A:292:THR:HG23	2.12	0.48
1:A:251:THR:HG23	6:A:1315:HOH:O	2.14	0.48
1:A:463:ALA:HB1	1:A:469:GLU:CB	2.44	0.48
1:A:358:HIS:HD2	1:A:359:SER:O	1.97	0.47
1:A:302:ASN:HD22	1:A:302:ASN:C	2.23	0.47
1:A:383:ARG:HD2	1:A:383:ARG:O	2.15	0.47
1:A:395:ASN:HD21	1:A:431:THR:CG2	2.27	0.47
1:A:135:ARG:CD	6:A:1605:HOH:O	2.58	0.46
1:A:125:ARG:HD3	6:A:1523:HOH:O	2.16	0.46
1:A:450:HIS:HE1	6:A:1228:HOH:O	1.99	0.46
1:A:439:VAL:CG2	1:A:458:ILE:HD11	2.46	0.45
1:A:82:THR:CG2	1:A:357:ASP:O	2.65	0.44
1:A:143:VAL:HG12	1:A:307:PHE:HB3	1.98	0.44
1:A:302:ASN:HD22	1:A:303:PRO:N	2.15	0.43
1:A:304:ARG:HG2	6:A:1506:HOH:O	2.17	0.43
1:A:302:ASN:HD22	1:A:304:ARG:H	1.63	0.43
1:A:77:VAL:HA	1:A:439:VAL:O	2.18	0.42
1:A:135:ARG:HD2	1:A:469:GLU:CA	2.43	0.42
1:A:262:VAL:O	1:A:263:THR:CB	2.67	0.42
1:A:395:ASN:HD21	1:A:431:THR:HG21	1.84	0.42
1:A:389:THR:O	1:A:392:LEU:CD2	2.67	0.42
1:A:84:ASN:HD21	1:A:91:ASP:H	1.66	0.42
1:A:458:ILE:HG22	1:A:462:MET:HE2	2.02	0.42
1:A:259:ASP:HA	1:A:260:PRO:HD2	1.94	0.42
1:A:260:PRO:O	1:A:261:SER:HB3	2.20	0.41
1:A:296:LEU:HD13	1:A:308:LEU:HD22	2.03	0.41
1:A:469:GLU:CB	1:A:470:PRO:HD2	2.49	0.41
1:A:155:SER:N	1:A:156:PRO:HD2	2.35	0.41
1:A:333:MET:HE2	6:A:1459:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:HIS:CD2	6:A:1115:HOH:O	2.71	0.41
1:A:148:THR:HG23	1:A:288:LEU:HG	2.01	0.41
1:A:392:LEU:HD23	6:A:1051:HOH:O	2.20	0.41
1:A:322:SER:O	1:A:420:ARG:HA	2.21	0.41
1:A:174:VAL:O	1:A:179:ARG:NH1	2.53	0.40
1:A:122:ASN:O	2:A:1000:NAG:H82	2.20	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1598:HOH:O	6:A:1598:HOH:O[3_655]	0.80	1.40
6:A:1133:HOH:O	6:A:1222:HOH:O[4_555]	1.91	0.29
6:A:1035:HOH:O	6:A:1399:HOH:O[3_655]	2.12	0.08
6:A:1133:HOH:O	6:A:1137:HOH:O[4_555]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	477/513 (93%)	460 (96%)	12 (2%)	5 (1%)	12 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	GLU
1	A	261	SER
1	A	473	ALA
1	A	262	VAL
1	A	361	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	377/408 (92%)	358 (95%)	19 (5%)	22 6

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	26	LEU
1	A	82	THR
1	A	90	PRO
1	A	91	ASP
1	A	132	VAL
1	A	180	GLN
1	A	228	LEU
1	A	245	ARG
1	A	268	LEU
1	A	288	LEU
1	A	292	THR
1	A	296	LEU
1	A	348	GLU
1	A	353	LEU
1	A	383	ARG
1	A	431	THR
1	A	475	ASP
1	A	476	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	84	ASN
1	A	153	HIS
1	A	162	HIS
1	A	180	GLN
1	A	189	GLN

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Mol	Chain	Res	Type
1	A	193	ASN
1	A	302	ASN
1	A	358	HIS
1	A	450	HIS
1	A	453	GLN
1	A	455	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PO4	A	1005	3	4,4,4	2.90	3 (75%)	6,6,6	3.73	5 (83%)
2	NAG	A	1000	1	14,14,15	1.64	4 (28%)	17,19,21	2.33	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1000	1	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1005	PO4	P-O4	-3.73	1.43	1.54
5	A	1005	PO4	P-O2	-3.13	1.45	1.54
2	A	1000	NAG	O5-C1	3.10	1.48	1.43
5	A	1005	PO4	P-O1	3.08	1.57	1.50
2	A	1000	NAG	O7-C7	-3.02	1.16	1.23
2	A	1000	NAG	C1-C2	-2.64	1.48	1.52
2	A	1000	NAG	C2-N2	2.34	1.50	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	NAG	C2-N2-C7	7.97	133.59	122.90
5	A	1005	PO4	O4-P-O3	6.27	127.42	107.91
5	A	1005	PO4	O4-P-O2	3.96	120.22	107.91
5	A	1005	PO4	O4-P-O1	-3.70	97.86	110.95
2	A	1000	NAG	C4-C3-C2	-3.04	106.56	111.02
5	A	1005	PO4	O3-P-O2	-2.75	99.36	107.91
5	A	1005	PO4	O3-P-O1	-2.37	102.56	110.95
2	A	1000	NAG	O7-C7-C8	2.29	126.13	122.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	NAG	C8-C7-N2-C2
2	A	1000	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1005	PO4	2	0
2	A	1000	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.